

allo-Cholanic acid, 3«beta»,7«alpha»-dihydroxy, Me-TMS

Other names:	3«beta»,7«alpha»-Dihydroxy-5«alpha»-cholanic acid, methyl ester, TMS
Inchi:	InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3
InchiKey:	FUVKOFYYHKWFJK-XHGKVCLCSA-N
Formula:	C31H58O4Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12O
Mol. weight [g/mol]:	550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpola	3223.00		NIST Webbook
rinpola	3223.00		NIST Webbook
rinpola	3223.00		NIST Webbook
ripola	3614.00		NIST Webbook
ripola	3614.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices
ripola:	Polar retention indices

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